now, $\underline{H = H_0 + V}$ vs $\underline{H_0}$

$$\Rightarrow \quad \mathcal{G}(z) = \frac{1}{z - H_0 - V} \quad \text{vs} \quad \mathcal{G}_0(z) = \frac{1}{z - H_0}.$$

By using the identity, $\dfrac{1}{A-B} = \dfrac{1}{A} + \dfrac{1}{A} B \dfrac{1}{A-B}$

$$= \frac{1}{A} + \frac{1}{A-B} B \frac{1}{A}$$

$$\Rightarrow \quad \underline{\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}} \;! \quad // \; A \equiv z - H_0, \; B \equiv V$$

$$\hookrightarrow \mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 V \mathcal{G}_0 + \cdots$$

… $\underline{\text{Born series}}$ "

$\Rightarrow$ Integral equation for the Green's function.

$$G(\vec{x}, \vec{x}') = G_0(\vec{x}, \vec{x}') + \int d\vec{s}\; G_0(\vec{x}, \vec{s})\, V(\vec{s})\, G(\vec{s}, \vec{x}')$$

// E is omitted.

(5) The Feynman Path Integral "

Dirac: $\exp\left[\frac{i}{\hbar}\underbrace{\int_{t_1}^{t_2} dt\, L_{\text{classical}}}_{= S \text{ (classical action)}}\right]$ corresponds to $\langle x_2 t_2 | x_1 t_1 \rangle$. ???

Feynman: $\exp\left[\frac{i}{\hbar} S\right]$ is proportional to $\langle x_2 t_2 | x_1 t_1 \rangle$. !

path integral

$$\Rightarrow \quad \langle x_N t_N | x_1 t_1 \rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)]\; e^{\frac{i}{\hbar} S[x(t)]}.$$

- A single free particle in 1D (t-indep.)

$$H = \frac{\tilde{p}^2}{2m} + V(\tilde{x}, \cancel{t}) \equiv T(\tilde{p}) + V(\tilde{x})$$

- We want to compute

$$\underset{\equiv (x_b t_b)}{K(b,}\ \underset{\equiv (x_a t_a)}{a)} = \langle x_b | \mathcal{U}(t_b, t_a) | x_a \rangle \, \Theta(t_b - t_a)$$

- Recipes of the path integral representation:

① breaking the evolution from a to b into a large sequence of K small forward steps in time of duration τ by means of the composition property for $\mathcal{U}$;

② evaluating each small step explicitly;

③ Showing that these steps sum to the form $\sum_P e^{\frac{i}{\hbar} S}$, where S is the classical action for some path P composed of linear segment from a to b;

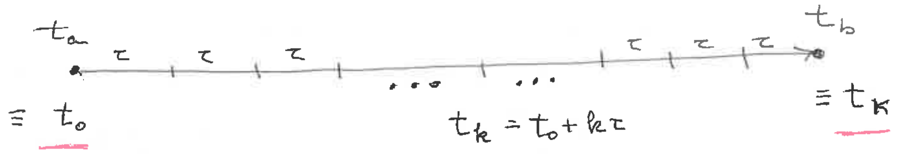
(④ Taking the limit, $\tau \to 0$, $K \to \infty$, $K\tau = t_b - t_a$.)

We assume this from the beginning!

→ Now, let's compute $K(b,a)$.

- Step 1: Break it into pieces.

$$K(b,a) = \langle x_b | \mathcal{U}(t_b, t_b - \tau) \cdots \mathcal{U}(t_a + 2\tau, t_a + \tau)\, \mathcal{U}(t_a + \tau, t_a) | x_a \rangle$$



NOTE: $K \equiv N$, $\tau = \Delta t$ in Sakurai.

$$k = 0, 1, \cdots, \frac{t_b - t_a}{\tau}$$

Let $x_a \equiv x_0$, $x_b \equiv x_K$ as well.

$$\Rightarrow K(b,a) = \int_{-\infty}^{\infty} dx_{K-1} \cdots dx_1 \, \langle x_K | e^{-\frac{i}{\hbar}H\tau} | x_{K-1} \rangle \cdots$$

$$\cdots \underbrace{\langle x_2 | e^{-\frac{i}{\hbar}H\tau} | x_1 \rangle}_{\text{a propagator } \langle x_2 t_2 | x_1 t_1 \rangle} \langle x_1 | e^{-\frac{i}{\hbar}H\tau} | x_0 \rangle .$$

= (a product of propagators) "

- Step 2: compute $\langle x_{k+1} t_{k+1} | x_k t_k \rangle$ by using that τ is small "

  (This is also hard because of "V").

  - ~~A~~ naive thought

    $$e^{-iH\tau/\hbar} \simeq 1 - \frac{i}{\hbar} H\tau \longrightarrow \text{a big error.}$$

    [a composition property breaks down in $\mathcal{O}(\tau^2)$.]

  - The Better one : the Suzuki-Trotter decomposition "

    $$e^{-\frac{i}{\hbar}H\tau} \simeq e^{-\frac{i}{\hbar}T\tau} \, e^{-\frac{i}{\hbar}V\tau} \quad \text{when } \tau \text{ is small.}$$

    → perfect unitarity !

    || NOTE : Baker-Campbell-Hausdorff (BCH) theorem.

    $$e^A e^B = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}\left([A,[A,B]] - [B,[A,B]]\right) \cdots \right)$$

$$\Rightarrow \langle x_{k+1} | e^{-\frac{i}{\hbar}H\tau} | x_k \rangle \simeq \underbrace{\langle x_{k+1} | e^{-\frac{i}{\hbar}T\tau} | x_k \rangle}_{\text{a free-particle propagator}} e^{-\frac{i}{\hbar}V(x_k)\tau}$$

$$= \sqrt{\frac{m}{2\pi i \hbar \tau}} \exp\left[\frac{i}{\hbar} \left(\frac{m(x_{k+1} - x_k)^2}{2\tau} - \tau V(x_k) \right) \right] .$$

Step 3: It's done.

$$K(b,a) = \lim_{\substack{\tau \to 0 \\ K \to \infty \\ (\| K\tau = t_b - t_a)}} \left(\frac{m}{2\pi i \hbar \tau} \right)^{\frac{1}{2}K} \int_{-\infty}^{\infty} dx_{K-1} \cdots dx_1 \,.$$

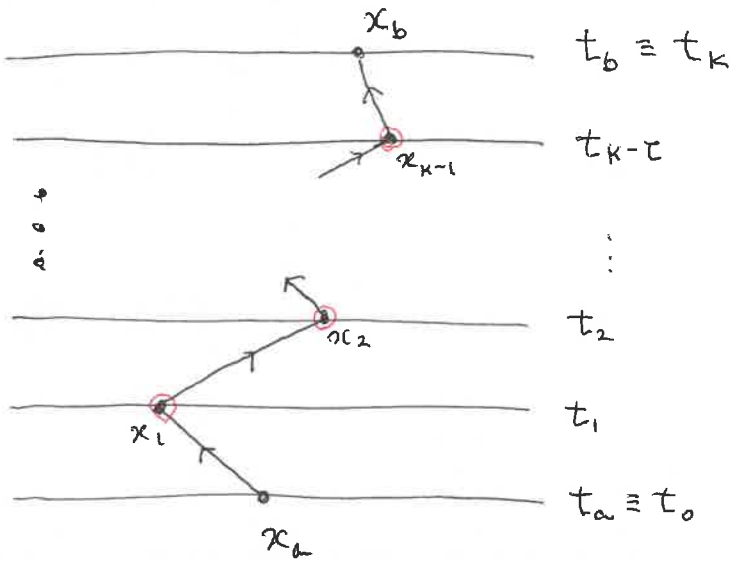
$$\cdot \exp \left[\frac{i\tau}{\hbar} \sum_{k=0}^{K-1} \left(\frac{m}{2\tau^2} (x_{k+1} - x_k)^2 - V(x_k) \right) \right] .$$

→ It can be evaluated by using PIMC.

(path-integral Monte Carlo.)

• Meaning and a shorter form.

Integrand : a "path". $\int \cdots \int$ = sum over the paths.



☆ The beads ⊙ move freely, but feel the adjacent beads.

☆ The links ↗ are just like springs!

$\left(\frac{m}{2\tau^2} (x_{k+1} - x_k)^2 \right)$: a harmonic term!

One can also see

$$\lim_{\tau \to 0} \left(\frac{m}{2\tau^2} (x_{k+1} - x_k)^2 - V(x_k) \right) = \frac{1}{2} m \dot{x}_k^2 - V(x_k)$$

$$= L_{\text{classical}} (x_k, \dot{x}_k ; t_k) .$$

NOTE:

$$\frac{dx}{dt} = \lim_{\Delta t \to 0} \frac{\Delta x}{\Delta t}$$

So it's classical!

$$\Rightarrow \lim_{\substack{\tau\to 0\\ K\to\infty \\ K\tau = t_b - t_a}} \tau \sum_{k=0}^{K-1} L_{\text{classical}}(x_k, \dot{x}_k ; t_k) = \int_{t_a}^{t_b} dt\, L(x, \dot{x}; t)$$

$$= S_{ba}[x(t)] \leftarrow \text{Classical Action "for } x(t)\text{"} ☆$$

$$\Rightarrow K(b,a) = \int_a^b \mathcal{D}[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right).$$

$$\| \quad \int_a^b \mathcal{D}[x(t)] \equiv \lim_{(\cdots)} \left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{K}{2}} \int_{-\infty}^{\infty} dx_{K-1} \cdots dx_1$$

(6) Free-particle Path Integral (as an example.)

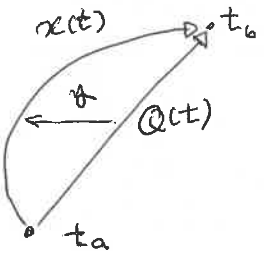
$$K(b,a) = \lim_{\tau\to 0} \left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{K}{2}} \int_{-\infty}^{\infty} dx_{K-1} \cdots dx_1 \exp\left[\frac{i\tau}{\hbar} \sum_{k=0}^{K-1} m \frac{(x_{k+1}-x_k)^2}{2\tau^2}\right].$$

: Some trouble occurs at fixed beads - x_0, x_K.

→ Let's substract the classical "path" from $x(t)$.

$\equiv Q(t)$: fixed.

→ devations $y(t) = x(t) - Q(t)$



$$\Rightarrow \sum_{k=0}^{K-1} (x_{k+1} - x_k)^2 = \sum_{k=0}^{K-1} (\underbrace{Q_{k+1} - Q_k}_{\text{const. (velocity = const.)}})^2$$

$$+ \sum_{k=0}^{K-1} (y_{k+1} - y_k)^2$$

$$\cancel{+ 2\sum_{k=0}^{K-1} (\underbrace{Q_{k+1} - Q_k}_{=\text{const.}})(y_{k+1} - y_k)} \rightarrow 0$$

$$\therefore \Sigma \Delta y = 0.$$

$$\Rightarrow S[x(t)] = \frac{m}{2} \int_{t_a}^{t_b} dt \left[\dot{Q}^2(t) + \dot{y}^2(t)\right]$$

and

$$\int_{t_a}^{t_b} dt\, \frac{1}{2} m \dot{Q}^2(t) = \frac{1}{2} m \cdot \left(\frac{x_b - x_a}{t_b - t_a}\right)^2 \cdot (t_b - t_a) = \frac{1}{2} m \frac{(x_b - x_a)^2}{t_b - t_a}$$

$$\equiv S_{cl}(b,a) \leftarrow \text{along classical "path"}$$

$$\Rightarrow K(b,a) = \int_a^b \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}$$

$$= F(t_b - t_a) \cdot e^{\frac{i}{\hbar} S_{cl}(b,a)}$$

where $$\underbrace{F(t_b - t_a)}_{} = \int_{t_a}^{t_b} \mathcal{D}[y(t)]\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{1}{2} m \dot{y}^2(t)} \quad \| \; y(t_a) = y(t_b) = 0 .$$

time translation invariant (free particle!)

- Evaluation of $F(t)$ $\quad \| \quad t_a = 0, \; t_b - t_a \equiv t .$

① Quick and easy, but specific. $\quad \| \; (y, t')$: a way point.

$$F(t) = \int_{-\infty}^{\infty} dy\, K(0,t\,;\, y, t')\, K(y, t'; 0, 0)$$

← composition property is used.

$$(x=0,\, t=0) \xrightarrow{\quad F \quad} (x=0,\, t=t)$$

$$(x=y,\, t')$$

$$= \int_{-\infty}^{\infty} dy\, F(t-t')\, e^{\frac{i}{\hbar}\frac{y^2}{t-t'}\cdot\frac{m}{2}}\, F(t')\, e^{\frac{i}{\hbar}\frac{y^2}{t'}\cdot\frac{m}{2}}$$

$$= F(t-t')\,F(t') \int_{-\infty}^{\infty} dy\, \exp\left[i y^2 \left(\frac{1}{t-t'} + \frac{1}{t'} \right) \frac{m}{2\hbar} \right]$$

$$= F(t-t')\,F(t') \sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t'(t-t')/t} .$$

↳ factored as :

$$\left[\sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t}\, F(t) \right] = \left[\sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t-t'}\, F(t-t') \right] \left[\sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t'}\, F(t') \right] .$$

$$\therefore \; F(t) = \sqrt{\frac{m}{2\pi i\hbar t}} \;\Rightarrow\; \underbrace{K(b,a) = \sqrt{\frac{m}{2\pi i\hbar (t_b - t_a)}}\; e^{\frac{i m (x_b - x_a)^2}{2\hbar (t_b - t_a)}}}_{}$$

as expected ...

③ Elaborative but general.

$$F(t) = \lim_{\tau\to 0} \left(\frac{m}{2\pi i \hbar \tau}\right)^{\frac{K}{2}} \int_{-\infty}^{\infty} dy_{K-1} \cdots dy_1 \exp\left[\frac{i}{\hbar} \cdot \frac{1}{2} m \sum_{k=0}^{K-1} \frac{(y_{k+1}-y_k)^2}{\tau}\right]$$

→ change of variables : $\eta_k = y_k \sqrt{\frac{m}{\hbar\tau}}$

$$\Rightarrow F(t) = \lim_{\tau\to 0} \left(\frac{m}{\hbar\tau}\right)^{\frac{1}{2}} \cdot \left(\frac{1}{2\pi i}\right)^{\frac{K}{2}} \int_{-\infty} d\eta_{K-1} \cdots d\eta_1 \, e^{\frac{i}{2} \sum_{k=0}^{K-1} (\eta_{k+1}-\eta_k)^2}$$

: This is just a multidimensional Gaussian integral.

$$* \int d^n x \, e^{-\frac{1}{2} \vec{x}^T A \vec{x}} = \sqrt{\frac{(2\pi)^n}{\det[A]}}$$

use the identity,

$$\sum_{k=0}^{K-1} (\eta_{k+1}-\eta_k)^2 = \vec{\eta}^T \cdot A \cdot \vec{\eta}$$

$\vec{\eta}^T = (\eta_1, \cdots \eta_k \cdots, \eta_{K-1})$

$\eta_0 = \eta_K = 0$

where $A = \begin{pmatrix} 2 & -1 & 0 & \cdots \\ -1 & 2 & -1 & \cdots \\ 0 & -1 & 2 & -1 \\ \vdots & & -1 & 2 & -1 \\ & & & \ddots & \ddots \end{pmatrix}$ "Laplacian matrix"

(K−1 by K−1 matrix)

→ easy to diagonalize : $A = U \tilde{\lambda} U^{+}$

↳ eigenvalues.

→ change of variables $\vec{\xi} = U^{+} \vec{\eta}$

$$\Rightarrow F(t) = \lim_{\tau\to 0} \sqrt{\frac{m}{2\pi i \hbar\tau}} \prod_{k=1}^{K-1} \int_{-\infty}^{\infty} \frac{d\xi_k}{\sqrt{2\pi i}} e^{\frac{i}{2} \lambda_k \xi_k^2}$$

$\vec{\eta}^T A \vec{\eta} = \vec{\xi}^T \tilde{\lambda} \vec{\xi} = \sum_k \lambda_k \xi_k^2$

$$= \lim_{\tau\to 0.} \sqrt{\frac{m}{2\pi i \hbar \tau \prod_{k=1}^{K-1} \lambda_k}}$$

$$\therefore F(t) = \lim_{\substack{\tau\to 0 \\ K\to\infty \\ \tau K = t}} \sqrt{\frac{m}{2\pi i \hbar \tau \det[A]}}$$

and we know that $\det[A] = K$ //

↳ reproduces $K(b,a)$